Report of the University of Chicago Review Committee for the Materials Science Division at Argonne National Laboratory

Elihu Abrahams
Rutgers University

David Bishop
Lucent Technologies

Susan Coppersmith
University of Wisconsin-Madison

Zachary Fisk
University of California, Davis

Hubert Gasteiger
General Motors Corporation

Allen Goldman (Chair)
University of Minnesota

Stuart Parkin
I.B.M Corporation

Caroline Ross
Massachusetts Institute of Technology

Rhonda Stroud
Naval Research Laboratory

26 – 28 February 2006

Executive Summary

The Materials Science Division (MSD) at Argonne National Laboratory has an exceptional record of scientific achievements, which are nationally and internationally recognized. Division personnel have achieved the highest levels of distinction in science in the form of prestigious international awards. Some of the groups in the division are clearly world leaders in their fields. The review committee was impressed with the exceptional leadership of Dr. George Crabtree.

The MSD is an extremely broad basic science enterprise engaged in areas that are important challenges for fundamental science including the discovery of new materials with unusual physical properties, high temperature superconductivity, catalysis, and with external support from the National Aeronautics and Space Administration (NASA) in probing the evolution of matter in the galaxy. It is actively engaged with problems that are on emerging frontiers, such as work on biomolecular materials and the development of quantum computing. Many of the research directions intersect strongly with the strategic objectives of the DOE Office of Basic energy Sciences (BES). The MSD, although not having a detailed long-range plan, has a well-defined, and demonstrably effective, strategy for identifying and supporting strategic opportunities for high impact programs and should thus be able to sustain its vigorous contributions. The committee recommends that this strategy be made available to all of the staff.

A long tradition of the Division and Argonne National Laboratory is that "science drives facilities and facilities drive science." The committee is concerned that recent organizational changes in DOE have put this paradigm at risk in some cases. In particular the separation of facilities from science in DOE management has introduced barriers between science and facilities, which were not present in the recent past. The panel recommends that special care be taken by the management to ensure the synergistic interaction between science and facilities continues at the laboratory. In the matter of the Center for Nanoscale Materials (CNM), the committee is concerned that there be coordination of hiring and program development in areas of nanoscience, between Chemistry, MSD and CNM. Regular consultation at the directors' level could ensure such coordination. In addition it is important that there be no barriers to joint projects, and that there be plans for managing joint projects.

Although a basic science enterprise, recently there has been a spin-off company formed to exploit ultrananocrystalline diamond technology developed in the Division. This appears to be a successful approach and we encourage MSD to continue to enable their staff to pursue applications-driven research according to their interests. The panel recommends that the Division attempt to enhance the impact of its science on industry by conducting industrial outreach. It feels that open communication of scientific advances to an industrial audience is extremely valuable. It does not recommend a focus on the control of intellectual property.

A key to many of the new initiatives of the Division is the success of junior staff working in interdisciplinary or cross-disciplinary areas. Mentoring and career guidance of junior staff by senior staff is particularly important to ensure the success of these activities. The committee recommends that each junior staff member receive adequate mentoring by his/her manager or another senior staff member.

I. **INTRODUCTION**

The Materials Science Division at Argonne National Laboratory has been a leader in numerous areas of science over the years. This has involved a combination of sophisticated techniques for the fabrication of materials, state of the art techniques of theoretical and experimental physical and chemical investigation, and simulation. The success of the Division has been due in part to its synergistic relationship with some of the unique facilities at Argonne such as the Intense Pulse Neutron Source and the Advanced Photon Source. Science in the Division has been an important driver for the development of these machines and their instrumentation. The Division's leadership position in fundamental international science has been sustained under the directorship of Dr. George Crabtree, who has provided both superb scientific leadership and excellent management. In the committee's interactions with staff, it was clear that there is much enthusiasm for the work of the Division, and that overall morale is very high.

This report is based on what was learned during a two-day review of the activities of the Division, which was held at Argonne National Laboratory from the evening of 26 February, through late afternoon of 28 February 2006. During this review the Committee was briefed by the managements of the Laboratory and the Division, met with early career scientists, heard numerous technical talks, and viewed significant numbers of posters at which there were opportunities for substantive discussions. The schedule of the Review is attached as Appendix A.

This report is organized in the following manner: the first section contains a direct response to the Committee's Charge. This is followed by brief evaluations of the programs that were presented in the review. Appendix B contains an outline of the strategy and tactics employed by the Division to guide its programmatic development. The charge to the Committee is supplied as Appendix C.

II. RESPONSE TO THE CHARGE

In this section the Committee's responses to the charge posed by the University of Chicago management are presented. The specific issues raised in the charge are given in bold italics.

Do the Division's research activities and achievements serve to advance the laboratory and DOE missions? Evaluate and benchmark the quality of the science programs, discussing both divisional strengths and challenges.

The Committee was unanimous in the view that the Division's research activities and achievements serve to advance the laboratory and DOE missions. This is evidenced by numerous publications in high impact journals, invitations to important conferences, and success in securing funding for research. In many areas of activity the programs of the Division are world leaders. Details of the Committee's opinion regarding various activities of the Division are found in Section III. Several programs address what might be termed the *grand challenges for fundamental science*, the mechanism of high-T_c superconductivity, the atomic and molecular basis of catalysis, and with external support, aspects of the origin of the universe. Other programs such as the activities in biomolecular materials, and molecular spin qubits for quantum computing recognize emerging science frontiers.

The division has also played an important role in helping BES shape its energy mission through its participation in the development of workshops such as those on the hydrogen initiative, superconductivity, and catalysis.

Evaluate the Materials Science Division's strategic plan including: strategic objectives, timeline hiring plans, resource requirements (laboratory, DOE, other); strategies for exploiting other funding opportunities, expected outcomes, measures of success, strategies for addressing future challenges and growth opportunities, concepts for working with the University of Chicago and other academic institutions and for engaging industry.

The Laboratory's long-range plan prepared for BES, which was supplied as background material, contained a brief discussion of the plans for the Materials Sciences Division. There is no detailed long-range plan such as was recommended by the previous Committee. The Division held a retreat, which served as a planning exercise, about two years ago, but no formal document was produced. The Committee did receive a very clear written statement from the Division Director, which impressively set out strategic goals and tactics for achieving them. In an environment in which the Division is responding to a changing array of basic science opportunities in a framework in which the strategic goals of the funding agency may also be shifting, flexibility is critical and long-range plans tend to have a short life. The document provided indicated how MSD went about identifying strategic opportunities for high impact programs, the approach to the selection of target programs from strategic opportunities, and the mechanisms for initiating programs. It included a discussion of the relationship with BES, the approach to the recruitment of new hires, how the division responded to BES calls, how unsolicited proposals to BES and other agencies were generated, and the mechanism for preparing proposals. We were also provided with a summary of programs initiated in the last three years, the processes of program evaluation, and the evaluation of scientific personnel.

It is clear that a *de facto* plan and approaches to operation and decision-making are in place. A document similar to the one provided to the committee should be available to the staff, so that they can have a clear picture of how directions for the Division are set. We have included for completeness the materials provided to us in the review in Appendix B.

An important aspect of the work of the Division that is especially important to its long-term scientific success is the continuing development of scientific personnel of the highest quality. In speaking to staff, particularly junior staff, the Committee found that morale is generally high. However, some staff commented that junior scientists might have difficulty in initiating their programs because they are not equipped with start-up funds, so mentoring and career guidance of junior staff by senior staff is particularly important. The committee recommends that each junior staff member receive adequate mentoring by his/her manager or another senior staff member.

MSD has not simply relied on its historical strengths in materials physics but has recently begun forays into new areas such as biomaterials, catalysis and multi-scale modeling. Evaluate financial, human and physical resources for maximizing both traditional lines of

research and these growth directions. Many of these new efforts require expertise in areas not traditionally residing in the Division. Evaluate the plan for building this expertise either internally or through strategic partnerships.

During the review, several activities were presented as new initiatives. The various activities all appear to have the potential for maturing into high impact programs consistent with the basic science focus of the Division and the goals of BES.

In Situ Studies of Thin Film Oxide Heterostructures

Dr. Petford-Long, a strategic new hire, is tasked with spearheading the effort in Lorentz microscopy, and leading the interfacial materials group. She clearly envisions strong partnership between oxide materials growth and properties characterization, matching a well accessorized sputter-MBE growth facility, with *in situ* x-ray and TEM characterization. Her position outside the Electron Microscopy Center may help foster the growth of basic science-driven, as opposed to facilities-driven, microscopy, as long as she does not face serious institutional barriers in managing the proposed aberration-corrected Lorentz microscope. Her development of the partnership with Hummingbird Scientific (Eric Stach) to optimize *in situ* TEM characterization of electrical properties is particularly exciting.

Catalysis: The mechanistic work in Electrocatalysis/Interfaces in Electrocatalysis is cutting-edge, using both advanced *ex-situ* and *in-situ* methods as well as striving to develop a novel in-situ TEM method (We applaud the plan to hire a microscopist specifically for catalysis work). In order to strengthen the program in electrocatalysis and solid/liquid interfaces, we recommend that a plan be established which incorporates the MSD's expertise in materials synthesis and molecular modeling. The expected synergy may lead to an internationally unique center of electrocatalyst development. Outreach to industry should be encouraged, with the goal both of educating industry about recently developed novel materials/materials preparation methods and of defining materials development needs in various industries.

Membrane Catalysis: The project, in which an anodic alumina template is functionalized using atomic layer deposition, was well presented and offers exciting opportunities for precise tailoring of both catalyst geometry and surface chemistry. The demonstrated synergy between materials synthesis, molecular modeling, and the evaluation of catalytic activity is outstanding; similar collaborative approaches should be pursued in Electrocatalysis work.

Quantum Computing: The new activity to build a quantum computer using nitrogen atoms inside C_{60} molecules involves an interesting combination of methods and expertise from a variety of fields. This ambitious project is a high-risk activity requiring novel, sophisticated, and interdisciplinary research.

Biological Sciences: The work on self-assembly of actin/myosin systems and of swimming bacteria is an interesting foray into this important area of pattern formation in biological systems. In the longer term, it is important to deepen the connections of this work to the biological community.

Nanophotonics: The project on plasmonic routes to nanophotonics exhibited very nice results on the propagation of surface plasmons around holes in metal films produced by focused ion beams, and the collection of light in a waveguide. This is a very active area at present. There are ample opportunities for collaboration which would be mutually beneficial, e.g. with Scherer's group at the University of Chicago. This is a nice example of work by an individual (Ulrich Welp) coming out of an older area and taking up a totally new research direction.

Condensed Matter Theory: The efforts in condensed matter theory are of very high quality. The panel applauds the hiring of Konstantin Matveev. At the same time, considering the size of the experimental effort in the Division, we recommend that the group be increased by several people. The panel questions the wisdom of the administrative fractionalization of the theory effort, now divided into two groups: Condensed Matter Theory and the Materials Theory Institute, neither of which have "critical mass." The Visitors Program administered by the Materials Theory Institute, discussed in the next section, has done well in bringing in excellent researchers and care should be taken to insure that that program includes activities of the Condensed Matter Theory group.

Digitally Engineered Magnetic Heterostructures: The new project concerning digitally engineered magnetic oxide heterostructures is currently using oxide MBE growth facilities in Jim Eckstein’s group at the University of Illinois at Urbana-Champaign, but has a proposal pending for the development of a novel thin film oxide MBE capability within the CNM/ MSD. This capability, which the committee supports strongly, would allow for the growth of thin film structures in which the composition and layer thicknesses would be controlled to within very tight tolerances over relatively large areas, which would make possible advanced characterization and highly reproducible structures.

The MSD has recognized the benefit from greater awareness and exploitation of the potential applications that arise from its science efforts. Has the Division determined an appropriate balance between fundamental science and applications? Evaluate the plan for achieving this balance.

The committee appreciates that the emphasis of the DOE BES is on basic science. This activity is the traditional strength of the Division, and should remain so. The Division has been developing applications-driven research funded through additional sources, with some notable successes such as the formation of a company to commercialize diamond films. The pursuit of applications-driven research is a bottom-up activity carried out by those MSD scientists who are most interested in doing it, without being driven by the Division management. This appears to be a successful approach and we encourage MSD to continue to enable their staff to pursue applications-driven research according to their interests. These activities, in total, will constitute a small fraction of the overall research activities carried out by the Division, consistent with the basic research-oriented culture of the Division.

The panel recommends that the Division attempt to enhance the impact of its science on industry by conducting industrial outreach. This could be accomplished in part by hosting short-term industrial visitors and organizing workshops targeted at industrial participants. The panel feels that open communication of scientific advances to an industrial audience is extremely valuable. It does not recommend a managerial push to encourage patents or to focus on the control of intellectual property. Nevertheless, the filing of patent applications should be supported speedily when it is clearly required in order to disclose detailed information to interested industries. (In industrial practice, the filing of patent applications should not require more than one month.)

One of the unique features of the MSD is its close coupling with Argonne's scientific facilities such that science drives facilities and facilities drive science. Evaluate the management plan for achieving this with respect to neutron and x-ray scattering a well as electron microscopy efforts.

The committee resonated very strongly with the idea that science drives both large- and small-scale facilities and in turn these facilities drive compelling new science. The committee is concerned that recent organizational changes in DOE have put this paradigm at risk in some cases. In particular the separation of facilities from science in DOE management has introduced barriers between science and facilities that were not present in the recent past and are not conducive to productive science. The panel recommends that special care be taken by the management to ensure the synergistic interaction between science and facilities continues at the laboratory. In the matter of neutron and x-ray scattering activities, there is a long history of coordination of activities involving materials growth and scientific investigation with technique development. This appears to be continuing with the proposed work on diffuse scattering and the development of spin echo resolved grazing incidence scattering (SERGIS) of neutrons. The latter should indeed provide an opportunity for addressing issues in soft matter and biomembranes. The hiring of additional personnel in this area will be crucial to ensuring its success. The SERGIS activity should help to secure the position of the Division in its role of developing instrumentation driven by science. It will also help secure participation in SNS.

The microscopy center should be commended for developing a strategic plan that balances far-reaching instrument development tasks Transmission Electron Aberration Corrected Microscopy (TEAM) with near-term *in situ* advanced studies, and making critical new hires to support these goals. The center clearly recognizes that close coordination with in-house expertise in materials growth can provide a competitive edge for basic science funding, over strictly technique development-driven user facilities. The facilities maintenance costs (service contracts) will escalate dramatically with the arrival of the new microscopes, and a clear line of funding from DOE headquarters is needed to support these facilities.

Although not directly addressed in this section of the charge, the development of the Center for Nanoscale Materials (CNM) is particularly important, because it is a significant opportunity for Argonne and especially the Division. Many of the research activities of the Division are within the broad area of nanoscience. It is important the CNM be a partner with the Division (and the Chemistry Division) in its research activities. We are concerned that there be coordination of hiring and program development between Chemistry, MSD and CNM. The same issue of science driving facilities is important. To insure that this coordination take place, we propose that there be regular consultation at the directors' level, that there be no barriers to joint projects, and that there be plans for managing joint projects.

III. DISCUSSION OF PROGRAMS

Superconductivity and Related Areas: Vortex Physics, Strongly Correlated Electron Systems

The work being carried out on superconductivity in the MSD is an example of some of the very best vortex physics research in the world. The group has had a leading role since the discovery of high-T_c superconductivity almost twenty years ago and continues to impress with the quality and quantity of their work. In their imaging and transport work, key and important ideas are being tested and new concepts put forth and made part of the scientific mainstream. This group, which is accompanied by a strong theoretical effort, is one of the best known and most prolific to be found in a DOE lab and is a role model. The challenge for any DOE research program is to do world-class research in areas of frontier science of potential technological interest and do it in a way that enhances the prestige of the parent institution. This program succeeds admirably.

One of the most important frontier problems in condensed matter physics is that of strongly correlated electron systems. One of the oral presentations addressed a key aspect of this problem directly: J.C. Campuzano is a world leader in the field of photoemission who has half-time appointments at ANL and UIC. He presented some of his latest work on the pseudogap phase of high-temperature cuprate superconductors. This is leading edge physics of importance to the field. His quite unexpected and stimulating result, using angular-resolved photoemission (ARPES) techniques, is that the characteristics of the electronic structure in the pseudogap phase scale with a characteristic temperature that varies with the doping and their temperature dependences show no sign of the proximate superconducting transition temperature.

Campuzano leads a remarkably successful group whose research commands world attention. He uses recent technical advances in ARPES to explore systems involving strongly correlated electrons. There is a very strong and fruitful interaction with the Condensed Matter Theory group of M.R. Norman, himself a leading theorist with a superlative international reputation. Thus, although small, the ANL effort in strongly correlated materials is something of which the laboratory can feel quite proud.

Dr. Konstantin Matveev recently joined the Division. He brings to Argonne expertise in low-dimensional electron systems, an area that plays a very important role in the general problem of the physics of strongly correlated electrons. In fact, one-dimensional (1D) interacting electrons are a canonical example of unusual behavior arising because of strong interactions. K. Matveev addressed an interesting problem in the electrical transport of one-dimensional ballistic “quantum” wires. Briefly, when the electron density is low, the interactions are especially important and an unexpected plateau (at one-half the “standard” value) in the conductance as a function of density has been observed in experiment. Matveev is a leading theorist in the field and he presented his theory of this effect based on the observation that at sufficiently low density, the electron system should form a Wigner crystal.

The significance of this work lies in at least two areas. One is the theory of 1D interacting electrons, which at low density now must be extended beyond the conventional (“Luttinger liquid”) picture of spin-charge separation. Another is the possibility that this development offers an opportunity for developing insights into an important forefront problem, that of interacting electrons in two dimensions (2D). The 2D problem involves a possible experimentally observed metal-insulator transition for electrons at low density in proximity to a 2D Wigner crystal phase, and it has proved extremely difficult to analyze.

Nanomagnetism

The nanomagnetism group within the MSD at Argonne has had a long history of outstanding scientific accomplishments that continues today. The group has continually evolved over the past ten years or more to keep pace with the world's best groups in this field and the group remains highly competitive internationally. In just the past year the group has published outstanding results on non-local spin transport in spin-valve structures, the dynamics of vortex pairs in ferromagnetic elliptical dots of permalloy, investigated using a new microwave reflectivity setup developed within the MSD, work on novel bio-functionalized magnetic particles, and work on time-resolved magnetic imaging using photoemission electron microscopy at the Advanced Light Source. The group uses, to great advantage, the scattering capabilities at the APS. A new project concerning digitally engineered magnetic oxide heterostructures, mentioned earlier, is currently using oxide MBE growth facilities in Jim Eckstein's group at the University of Illinois but has a proposal pending for the development of a novel thin film oxide molecular beam epitaxy (MBE) capability within the CNM/ MSD. This capability, would allow for the growth of thin film structures in which the composition and layer thicknesses would be controlled to within very tight tolerances over relatively large areas that would make possible advanced characterization and highly reproducible structures. The interaction with the materials synthesis group in the Division, where there is deep understanding of the properties of complex materials, which can serve as a guide to controlled growth, is a unique aspect of this effort.

The nanomagnetism group would particularly benefit from the hiring of several of its outstanding visiting scientists, especially, Kristen Buchanan, K. Guslienko and Anand Bhattacharya, all of whom are world-class.

Materials Synthesis

Materials synthesis both motivates and enables an important part of the research in the Materials Science Division. The Emerging Materials Group is primarily concerned with bulk materials synthesis and has a strong record, particularly in oxide materials. These include cuprate superconductors, manganites and frustrated layered oxides. Strong coupling exists between the materials experts, those measuring electronic and magnetic properties, and the neutron scatterers. An example of the effectiveness of this interplay can be seen in the optimization of T_c through careful quantified hydration of $Na_xCoO_{2-\delta.}\bullet yH_2O$ (y=4x) and the identification via neutron scattering structural studies that this optimization corresponds to the formation of a true hydrate rather than simply the intercalation of water. The work synthesizing crystals of the magnetically frustrated compound, $La_{1-x}Sr_xCoO_3$, has enabled discovery of short-range magnetic order at low temperature involving unusual spin-1 cobalt, an important addition to our knowledge in this interesting class of materials. Careful materials work in the layered manganites has led to revision of some of the accepted phase equilibria, work providing as well important reference for the interesting research in digital synthesis of complex oxides.

The decision to pursue synthesis of materials at high pressures has much promise and is not a capability possessed in many laboratories. The new effort in N-containing intermetallics will be able to extend considerably its phase space utilizing high pressures and has the potential for novel discoveries. An interesting thread which runs through the materials effort historically is the study of superconducting materials, and this continues to provide a surprisingly vigorous common ground for the scientific discourse of scientists with diverse background and experience. The spin-off of the ultrananocrystalline diamond activities is an unusual and innovative approach to commercialization within DOE, which may provide an important model for the future.

There is evidence of a high level of enthusiasm within the materials synthesis and related efforts, both in the staff and the postdoctoral fellows. A valuable strength of this effort is its wide range of collaborative interactions, both nationally and particularly internationally. Overall, their research effort is robust, highly competitive and commands justified international recognition. In view of the lack of competitiveness of the US on the international scale in materials synthesis, we recommend that serious consideration be given to adding several scientists to this group. In this case more effort could be placed both on development of new materials and on materials synthesis in support of the catalysis/electrocatalysis programs.

Modeling Complex Molecular Systems

There is a small but active and respected group working on modeling complex molecular systems. This group is developing new quantum chemistry techniques and applying them to systems of interest to the experimental groups working on novel catalytic materials. The work on electrocatalysis is relevant to the use of hydrogen as an energy source, and that on biomimetic energy conversion is relevant to new developments in solar energy.

Cosmochemistry

The Cosmochemistry group is a world leader resonant ion mass spectrometry. They are making critical contributions to basic astrophysical questions concerning the formation and evolution of the elements. The high quality of the work is well recognized within the larger cosmochemistry community, as evidenced by the success of the group in obtaining NASA funding and their role in the Genesis and Stardust missions. The sample analysis needs of these missions are likely to be opportunities for stable continuing funds over the next decade, however the larger NASA budget priorities are in flux. The opportunities for growth in NASA funding over the long term are uncertain. The group should be commended for developing strong connections with leading researchers at the University of Chicago and the Field Museum, as well as collaborations with other US and international institutions. There is an opportunity internally for stronger collaborations with the EMC to develop coordinated structure-isotope measurements for better constraint of stellar evolution and early solar system modeling.

Electrocatalysis/Interfaces in Electrocatalysis

The research programs in Electrocatalysis/Interfaces in Electrocatalysis (N. M. Marković and H.

You) represent complementary and cutting-edge activities, utilizing advanced ex-situ (e.g., UHV surface characterization) and in-situ (e.g., FITR, X-ray scattering, in-situ TEM cell) tools to gain insight into detailed catalytic mechanisms and solid/liquid interface structures. A particular highlight is the envisaged bridging of model surfaces with application-relevant high-surface area catalysts, ranging from well-defined single cyrstals via idealized nano-particle arrays all the way to nano-particles on conventional high-surface area supports.

This mechanistically focused experimental program could be further strengthened, however, by establishing a clear plan on how to incorporate the MSD's expertise and background in molecular modeling and materials development. The anticipated synergism between materials development, insight into detailed catalytic mechanisms, and molecular modeling could evolve into a unique center for the development of novel electrocatalyst at ANL/MSD. While some plans were presented how members of the Electrocatalysis/Interfaces in Electrocatalysis program might collaborate with outside groups, it remained unclear how it would interface with the materials synthesis and modeling groups within MSD and the new CNM.

Biohydrodynamics and Emergent Behavior of Active Bioparticles

Igor Aronson described research on the self-assembly of microtubules and molecular motors and on swimming bacteria. Aronson is an extremely active and energetic researcher investigating a broad class of problems in the area of nonlinear dynamics and complex systems, and this work originated because of his realization that there are interesting analogies between these problems and some of his previous work on the physics of granular materials. The behavior of the motors on microtubules leads to alignment of the microtubules, and there is an analogy between this alignment with the decrease of transverse momentum that occurs when particles collide inelastically. These are original, interesting, and useful theoretical connections. The committee recommends that the relations between this effort and other biologists both inside Argonne and beyond, be strengthened.

Novel Nanostructured Membrane Catalysts

The work described by P. Stair is a very promising approach to the development of catalytic surfaces within the pores of anodic alumina (AAO). There has been a great deal of development of AAO worldwide, such that the ordering, periodicity, and pore size can be well controlled, and this provides a good basis for this project. The atomic layer deposition (ALD) technique is relatively new but extremely flexible in its ability to deposit monolayers of a range of elements, oxides, nitrides, etc. Other workers have reported the combination of ALD with AAO, but the use here in catalysis is particularly promising because of the extensive control that is possible over both the surface chemistry and the pore diameter. There is no doubt that this project will lead to new developments, especially if combined with some of the other expertise on modeling, surface science and electrochemistry in the Division.

Materials Theory Institute

Valerii Vinokur described the activities of the Materials Theory Institute, in which visitors come to Argonne. This activity has generated many high-profile publications and has done a good job of improving the communication between researchers at Argonne and others around the world. This effort is largely focused on aspects of theory in the area of nanoscience. We wish to emphasize that Materials Theory is broader that this. With Abrikosov, Norman and Matveev, the Division also has a very strong presence in the physics of strongly correlated electron systems, which is a central area in contemporary condensed matter theory, and which is also strongly linked to experimental work in the Division. It is important to recognize contributions in this area in the allocation of resources. The Materials Theory Institute should be a very broad umbrella.

Quantum Computing with Electron Spins

This program is a new initiative investigating a possible quantum computer architecture using C_{60} molecules with a single nitrogen molecule inside each of them, with the spin from the nitrogen being the qubit. The molecules are to be attached to specific sites on DNA molecules, enabling control of the qubit spacing, and the interactions between qubits are to be controlled by applied gates made using high-resolution e-beam patterned electrodes and single-wall carbon nanotubes. The architecture involves alternating C (N^{15}) and C (N^{14}), the former for the barrier spins and the latter for the qubits; the scaffolding method using DNA specificity makes this possible. The readout is to be accomplished using a radio frequency-single electron spin transistor using a spin polarized break junction and by Electron Spin Resonance (ESR) done by Scanning Tunneling Microscopy (STM), which has been shown to have single spin resolution on a different system. The interdisciplinary team of researchers is strong, and it will be interesting to see how this extremely ambitious and challenging project progresses.

Appendix A-Agenda

Final

THE UNIVERSITY OF CHICAGO

Review Committee Meeting for
Argonne National Laboratory's ***Materials Science Division***
February 26, 27 & 28, 2006

AGENDA

Sunday, February 26, 2006
<u>Argonne Guest House (AGH), Building 460, Conference Room A</u>

5:30 p.m. Reception

5:45 p.m. Welcome and Introduction ....Sidney Nagel, Board of Governors Liaison

6:00 p.m. Dinner *(in Argonne Guest* ***– Dining Room***)

7:00 p.m. Overview from the Director of
Argonne National Laboratory..Robert Rosner

7:10 p.m. "Charge to the Committee" ....Allen Goldman, Chairman

7:20 p.m. Overview from the Deputy Associate Lab Director of Physical, Biological
& Computing Sciences of Argonne National Laboratory...................Luis Nunez

7:40 p.m. Overview of the Materials Science Division......... ……………..George Crabtree

8:40 p.m. Interface of the Center for Nanoscale Materials .... Eric Isaacs

9:00 p.m. Executive Session for Review Committee Members

9:30 p.m. Adjourn for evening

THE UNIVERSITY OF CHICAGO

Review Committee Meeting for
Argonne National Laboratory's ***Materials Science Division***
February 26, 27 & 28, 2006
AGENDA

Monday, February 27, 2006
Argonne Guest House (AGH), Building 460

7:00 a.m.	Breakfast with Early Career Staff, Conference Room "A"
7:45 a.m.	Transportation to Bldg. 212 (Meet in Lobby of Guest House)

Building 212, Conference Room A-157

Window on Core Research:

8:00 a.m.	Welcome .... George Crabtree
8:10 a.m.	Opportunities in Nanomagnetism .... Sam Bader
8:35 a.m.	Highlight: MagneticVortex Dynamics .... Kristen Buchanan
8:50 a.m.	Novel Vortex Phases in Cuprates, Meso-and-Nano-Superconductors .... Wai-Kwong Kwok
9:15 a.m.	Superconductivity in Cuprates .... Juan Carlos Campuzano
9:40 a.m.	Materials Synthesis; Strategies and Directions .... John Mitchell
10:05 a.m.	Highlight: Digital Synthesis of Complex Oxides .... Anand Bhattacharya
10:20 a.m.	***Break***
	Scattering Science:
10:40 a.m.	New Directions in Electron Scattering .... Dean Miller
11:05 a.m.	Probing Nanoscale Phenomena in Crystalline Materials Using Single Crystal Diffuse Scattering .... Stephan Rosenkranz
11:25 a.m.	Spin Echo Resolved Grazing Incidence Scattering of Neutrons; an opportunity for addressing issues in soft matter and biomembranes .... Suzanne Te Velthuis
11:45 p.m.	In-situ Studies of Thin Film Oxide Heterostructures .... Amanda Petford-Long
12:10 p.m.	***Working Lunch, Conference Room B-201 (Executive Session)***
1:40 p.m.	Modeling Complex Molecular Systems .... Larry Curtiss

THE UNIVERSITY OF CHICAGO

Review Committee Meeting for
Argonne National Laboratory's ***Materials Science Division***
February 26, 27 & 28, 2006
AGENDA

Monday, February 27, 2006 (Cont.)

Window on Translation to Applications:

2:05 p.m. Ultrananocrystalline Diamond: from the Laboratory to the Start-up... John Carlisle

2:25 p.m. Genesis and Stardust .... Michael Pellin

Window on New Initiatives:

2:45 p.m. Plasmonic Routes to Nanophotonics.. Ulrich Welp

3:05 p.m. Conductance of a Quantum Wire at Low Electron Density..... Konstantin Matveev

3:25 p.m. Materials Theory Institute: Quantum Mesoscopic Materials and Structures
.... Valerii Vinokour

3:45 p.m. ***Executive Session***

4:15 p.m. Transportation from Bldg. 212 to Bldg. 223 for **Poster Session**

4:30 p.m. Poster Session

6:30 p.m. Transportation from Bldg. 223 to **Freund Lodge**

6:45 p.m. U of C Hosted Reception/Dinner at Freund Lodge (by invitation only)

8:15 p.m. Transportation from Freund Lodge to Guest House, Bldg. 460

THE UNIVERSITY OF CHICAGO

Review Committee Meeting for
Argonne National Laboratory's ***Materials Science Division***
February 26, 27 & 28, 2006

Tuesday, February 28, 2006
Argonne Guest House (AGH), Building 460

7:00 a.m. Breakfast with Early Career Staff, Conference Room "A"
7:45 a.m. Transportation to Bldg. 212 (Meet in Lobby of Guest House)

Building 212, Conference Room A-157

8:00 a.m. Opening .... George Crabtree

New Initiatives:

8:10 a.m. Electrocatalysts Designed from Fundamental Principles..............Nenad Markovic

8:35. a.m Highlight: Studies of interfaces important in electrocatalysis ......Hoydoo You

8:50 a.m. Quantum Computing with Electron Spins...Frank Fradin

9:10 a.m. Biohydrodynamics and Emergent Behavior of Active Bioparticles
from Self-Assembling Microtubules to Swimming Bacteria ....Igor Aronson

9:30 a.m. Novel Nanostructured Membrane Catalysts.. Peter Stair

9:50 a.m. Executive Summary and Questions ....George Crabtree

10:10* a.m. *Break

10:30 a.m. Executive Session, Report Writing

12:00 p.m. Working Lunch, Conference Room A-157 (Executive Session)

1:00 p.m. Report Preparation, Conference Room A-157

2:30 p.m. Close-out with ANL Directorate............ Bob Rosner, Don Joyce, Kelly Mannsfeld

3:00 p.m. Close-out with ALD and Division Director(s) ....
...........Luis Nunez, George Crabtree, Michael Pellin, Dean Miller and Sam Bader

3:30 p.m. Adjourn

Appendix B

Materials Science Division

Strategic Planning and Implementation Activities

February 2006

MSD has identified six areas of strategic opportunity with potential for high impact research:

Science and materials for energy, to address the demand for doubling energy production by 2050 without deleterious effect on the environment or climate change
e.g. catalysis, biological and biomimetic energy conversion, basic research supporting hydrogen as an energy carrier and sunlight as an energy source.

Scattering science with electrons, neutrons and x-rays, to advance the frontier of materials science and develop new scientific capability for BES scattering facilities
e.g., Transmission Electron Aberration Corrected Microscopy (TEAM), single crystal diffuse scattering, spin echo resolved grazing incidence spectroscopy (SERGIS)

In situ experiments, to probe the real-time dynamics of physical, chemical, and biological phenomena
e.g. MOCVD epitaxial film growth, environmental TEM

Grand challenges of fundamental science, to create basic understanding of the behavior of materials
e.g., the mechanism of high temperature superconductivity, catalysis and control of chemical transformation

Emerging science frontiers, to explore opportunities for discovery of new fundamental phenomena
e.g., biomolecular materials, quantum computing, plasmonics, spintronics, ultra-fast (~femtosecond), ultra-small (~nanometer), complexity

Applications of MSD basic research, to translate MSD's discovery science to materials development
e.g., UNCD, hydrogen sensors, artificial retina, high temperature superconducting wires

New programs from among the strategic opportunities are selected by the following criteria:

Programs that address more than one strategic opportunity

Programs that achieve critical mass enabling world-class impact: talent, equipment, inspiration, resources

Areas of BES interest: basic materials research for energy needs- hydrogen, solar, superconductivity, solid state lighting, nuclear energy, . . .

Areas of other agency interest, e.g., artificial retina with Second Sight through Office of Biological and Environmental Research (DOE-BER), origin of matter in the universe through NASA

Programs selected for development within BES are launched using one or more of the following approaches:

Developing a relationship with BES. Examples are

Organizing “Basic Energy Needs . . .” workshops

Participating in BESAC Panel on Theory and Computation

Disseminating Workshop and Panel conclusions to scientific community, OSTP, and Congress

Discussion with BES of whitepapers for potential MSD full proposals

Recruitment of new hires coupled to unsolicited proposals to BES. Examples are

Konstantin Matveev for theory

Nenad Markovic for electrocatalysis

Amanda Petford-Long for electron microscopy and materials science

Response to BES calls. Examples are

Fundamental Research on the Oxygen Reduction Reaction, Hoydoo You

Transmission Electron Aberration Microscopy (TEAM), Dean Miller, Bernd Kabius

Atomic Scale Elemental Imaging in Three Dimensions, Bernd Kabius, Amanda Petford-Long

Unsolicited proposals to BES. Examples are (see below for details)

Digital Synthesis of Complex Oxides, Anand Bhattacharya, John Mitchell

Surface plasmonics, Ulrich Welp, Vitalii Vlasko-Vlasov

Hydrodynamics of physical and biological systems, Igor Aronson

Quantum computing, Frank Fradin

Electrocatalysis, Nenad Markovic

Argonne Lorentz TEM, Amanda Petford-Long

Diffuse scattering techniques and science, Stephan Rosenkranz, Ray Osborn

Granular conducting arrays, Valerii Vinokur, Andrei Lopatin

Proposals to funding agencies other than BES are developed with the following approaches:

Choose agencies with a history of funding PIs over the long term

Develop a relationship with the agency and its managers

Build large, long term programs

Examples are

Artificial Retina (Second Sight, through Office of Biological and Environmental Research, funded and continuing, $200K out of $1.2M program)

Nanomagnetism in viruses (Biosciences Division (ANL) through DARPA, funded and completed)

Development of high temperature superconducting wires for applications (Office of Electricity Delivery and Energy Reliability, $1M/yr, continuing)

UNCD cantilevers (DARPA, funded and continuing)

Trace element analysis of extra-terrestrial matter (NASA, $500K/yr, continuing)

Proposals are prepared by the following mechanisms:

Coordinated teams for preparing parallel proposals (up to six across Argonne) for the BES hydrogen, solar, and catalysis calls

Proposal teams of 2-5 PIs for unsolicited proposals

Iterative and interactive review outside the proposal team

Programs are evaluated by the following mechanisms:

Programs are evaluated in detail every three years in preparation for required DOE reviews. These reviews are done by external panels of peers drawn from the community, by mail and on-site, for each funded program (Field Work Proposal (FWP) in DOE language). The level of the DOE review is approximately equivalent to an NSF MRSEC review.

Programs are evaluated annually through the annual MSD individual performance appraisal review. The enclosed Performance Appraisal Form defines the criteria for evaluation. Program Development, Program Achievement, and Program Outreach are three of the four evaluation criteria. Scientists are evaluated on personal achievement (points 1-4) and on program achievement (points 5-9). Senior Scientists (Grade 709-710) and Group leaders are evaluated additionally on program effectiveness.

The following strategic programs have been initiated in the last three years:

Electronic properties of quantum wires: Konstantin Matveev, recruited and initial funding ($300K/yr) in 2003, additional funding in 2005 ($250K/yr)

Atomic and molecular basis of electrocatalysis: Nenad Markovic recruited and initial funding ($500K equipment, $300K/yr) in 2005, additional funding)for hydrogen proposal, Fundamental Research on Oxygen Reduction Reaction, Hoydoo You, $760K/yr) in 2005; proposal on electrolyte/substrate interfaces pending, $1M/yr (BES), proposal on specific catalysts for fuel cell reactions, in preparation to (EERE); proposal for evaluation of commercial catalysts with 3M, in preparation

Lorentz imaging of ferroelectric and magnetic phenomena: Amanda Petford-Long recruited and initial funding ($250K/yr) in 2005; collaboration with Nestor Zaluzec and Bernd Kabius; proposal for next generation Lorentz microscope pending to BES ($7M), white paper in preparation for science program

Quantum computing with electronic spins: Frank Fradin, John Schlueter, John Carlisle, Orlando Auciello, Tijana Rajh (CHM), funded in 2005, $400K/yr

Hydrodynamics of physical and biological systems: Igor Aronson and Ray Goldstein (University of Arizona), proposal pending to BES, $300K

Plasmonic routes to nanophotonics: Ulrich Welp, Vitalii Vlasko-Vlasov, proposal requested by BES

Granular conducting arrays: theoretical white paper submitted to BES, experimental white paper in preparation, collaboration with CNM, all in 2005

Genesis and Stardust: origin of elements in the universe, 4 separate proposals funded by NASA in 2005, ~$3M over five years

Digital synthesis of complex oxides: full proposal under review at BES, Anand Bhattacharya and collaborators, 2005

3D Chemical imaging: Bernd Kabius and Amanda Petford-Long, full proposal submitted to BES, seed funding of $150K/yr received, 2006

Diffuse scattering techniques and science: Stephan Rosenkranz, Ray Osborn, in collaboration with APS, Mathematics and Computer Science Division (MCS), white paper in preparation for BES call for mid-scale instrumentation

Appendix C – Charge

Charge to The University of Chicago Review Committee
for the Materials Science Division
at Argonne National Laboratory

February 26, 27 & 28, 2006

The Committee's charge is to evaluate the quality of the research, its relevance to DOE missions and national needs and the effectiveness and efficiency of research program management. Specific items for consideration include:

- Do the Division's research activities and achievements serve to advance the Laboratory and DOE missions? Evaluate and benchmark the quality of the science programs, discussing both divisional strengths and challenges.

- Evaluate the Materials Science Division's strategic plan including : strategic objectives, timeline; hiring plans, resource requirements (Laboratory, DOE, other); strategies for exploiting other funding opportunities, expected outcomes, measures of success, strategies for addressing future challenges and growth opportunities, concepts for working with the University of Chicago and other academic institutions, and for engaging industry.

    - MSD has not simply relied on its historical strengths in materials physics but has recently begun forays into new areas such as biomaterials, catalysis and multiscale modeling. Evaluate the financial, human and physical resources for maximizing both traditional lines of research and these growth directions. Many of these new efforts require expertise in areas not traditionally residing in the Division. Evaluate the plan for building this expertise either internally or through strategic partnerships.

    - The MSD has recognized the benefit from greater awareness and exploitation of the potential applications that arise from its science efforts. Has the Division determined an appropriate balance between fundamental science and applications? Evaluate the plan for achieving this balance.

    - One of the unique features of the MSD is its close coupling with Argonne's scientific facilities such that science drives facilities and facilities drive science. Evaluate the management plan for achieving this with respect to neutron and x-ray scattering as well as electromicroscopy efforts.